

**FINAL TECHNICAL REPORT****1 DEC 2000 TO 31 JUL 2004****NANOSCALE ENGINEERING OF MULTILAYER LAMINATES FOR HIGH TEMPERATURE APPLICATION****F49620-01-1-0092**

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<http://www.osu.edu/mse/~andersonp>**A. ABSTRACT**

The aim of the proposed research as stated in the original proposal is to understand how nanoscale laminates with optimal strength, ductility, and elevated temperature stability can be engineered through the selection of component chemistry, component layer thickness, and interfacial and grain boundary structure. The first effort is to develop computational tools to model the deformation and fracture processes in nanoscale laminates based on a well-known intermetallic system. The second effort is to apply the computational tools to at least one additional laminate system.

**B. RESEARCH OBJECTIVES**

- Fabricate nanoscale laminates based on the Ni-base  $\gamma/\gamma'$  system.
- Perform detailed characterization to understand deformation and fracture processes, as a function of layer thickness, interfacial structure, and crystal orientation.
- Develop computational tools based on the observed physical phenomena of dislocation motion and fracture, so that strength can be predicted as a function of layer thickness, interfacial structure, and crystal orientation.
- Fabricate and test the strength in at least one new material system. Candidate systems are high temperature multilayer laminates based on Ir/Ir<sub>3</sub>Zr or Ir/Ir<sub>3</sub>Nb, or novel material laminates based on a shape-memory NiTi alloy.
- Assess the ability of the computational tools to predict the strength in one or more material systems.

**C. APPROACH**

Nanoscale laminates based on the Ni-base  $\gamma/\gamma'$  system will be fabricated, characterized, and tested mechanically, in order to provide the necessary information for development and

calibration of computational tools. These tools will capture the relationship between microstructure and mechanical properties. Finally, the computational tools will be applied to at least one additional laminate system.

## D. RESEARCH ACTIVITIES AND RESULTS

### 1. Synthesis, Heat-treatment, Characterization, and Testing

A new set of nanoscale laminates consisting of alternating layers of  $\gamma$ -Ni(Al) and ordered  $\gamma'$ - $\text{Ni}_3\text{Al}$  phases was produced by ultra-high vacuum magnetron sputtering. The samples have a [001] texture along the interface normal and were produced with two values of bi-layer thickness,  $\Lambda = 50 \text{ nm}$  and  $300 \text{ nm}$ , and three volume fractions,  $f_{\gamma\text{-Ni(Al)}} = 0.4, 0.5, \text{ and } 0.6$ . The samples were then removed from the NaCl substrates, characterized with X-ray diffraction, and tested using nanoindentation in an "as-is" condition, after a 673K heat treatment for 36 hours, and after a 1073K heat treatment for 10 hours. Heat treatments were in an Argon environment.

*Principal Result 1: The magnitude of internal bi-axial stress in nanoscale laminates can be changed by up to +100%/-75% via heat treatment.*

Figure 1 shows that the stress magnitude, defined as the biaxial stress in  $\gamma$  minus that in  $\gamma'$ , is approximately 1 GPa for as-deposited, free-standing films. Heat treatment at 673K increases the stress magnitude by approximately 100% for both  $\Lambda = 50 \text{ nm}$  and  $300 \text{ nm}$  samples. Heat treatment at 1073K produces a 75% decrease in stress magnitude for  $\Lambda = 300 \text{ nm}$  samples. This new result suggests that "as-produced" nanoscale laminates may have nonequilibrium misfit dislocation densities that equilibrate only if a suitable heat treatment is applied.

*Principal Result 2: The hardness of nanoscale laminates is increased by increasing the internal bi-axial stress magnitude.*

Figure 1 shows that the relative nanohardness of nanoscale laminates increases with stress magnitude. The increase is more pronounced for  $\Lambda = 50 \text{ nm}$  compared to  $300 \text{ nm}$  samples. The result suggests a new strategy to optimize the strength of nanoscale laminates that has not been reported by researchers in the thin film community. References [L1, G3, G12] provide additional information related to Principal Results 1 and 2.

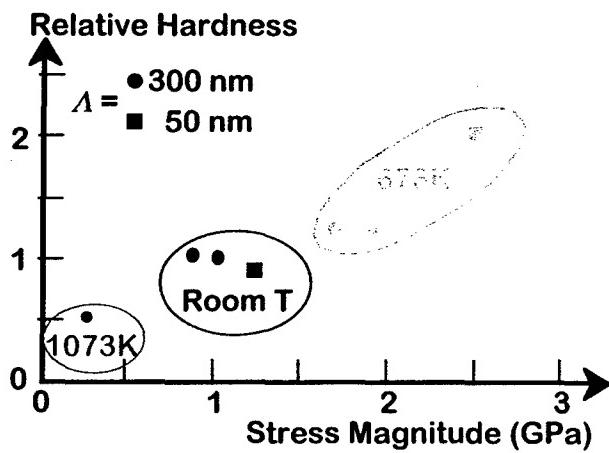


Figure 1: Relative Hardness vs stress magnitude (GPa) for  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  nanoscale laminates [L1].

## 2. Characterization of Microstructural Changes During Heat Treatment

Figure 2 shows cross sectional SEM images of  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  laminates with  $\Lambda = 300\text{nm}$  and  $f_{\gamma\text{-Ni(Al)}} = 0.4$ , in "as grown" condition, after a  $673\text{K}/36\text{ hr}$  heat treatment in Argon, and after a  $1073\text{K}/10\text{ hr}$  heat treatment in Argon. Figure 3 shows corresponding images for  $(\Lambda, f_{\gamma\text{-Ni(Al)}}, \text{heat treatment}) = (300\text{nm}, 0.6, 1073\text{K}/10\text{hr}), (50\text{nm}, 0.5, 1073\text{K}/10\text{ hr}),$  and  $(240\text{nm}, 0.5, 1373\text{K}/20\text{ hr})$ .

*Principal Result 3:  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  nanoscale laminates with  $\Lambda = 50\text{nm}$  to  $300\text{nm}$  and volume fractions  $f_{\gamma\text{-Ni(Al)}} = 0.4$  to  $0.6$  maintain a continuous laminate morphology in an Argon environment after a  $673\text{K}/36\text{ hr}$  heat treatment. After a  $1073\text{K}/10\text{ hr}$  treatment, thermal grooving of  $\gamma'$  layers is observed, particularly for samples with smaller  $\gamma'$  layer thickness; solutionizing is observed at 100 to 200K below that predicted for bulk samples, depending on  $\Lambda$  [L1, L2]. This novel result underscores a new, unique feature of  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  nanoscale laminates: the ability to undergo phase changes at temperatures significantly different from phase diagram predictions.*

References [L1, L2, G11, G12, G16, G18, G21, and G22] provide additional information related to Principal Result 3.

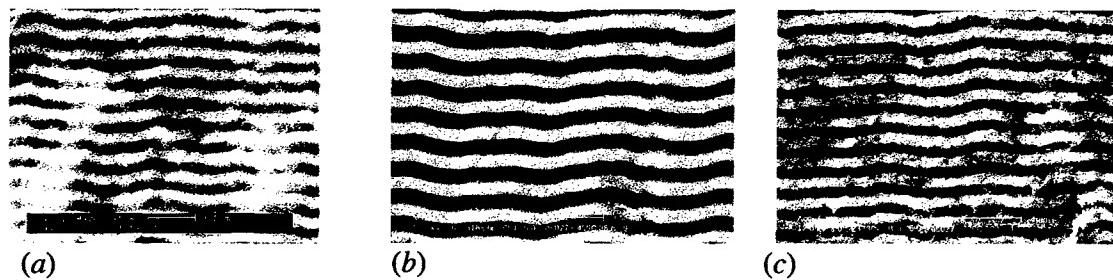


Figure 2: Cross sectional scanning electron microscope images of  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  multilayers with  $\Lambda = 300\text{nm}$  and  $f_{\gamma\text{-Ni(Al)}} = 0.4$  (a) in "as grown" condition, (b) after heat treatment in Argon at  $673\text{K}$  for  $36\text{ hours}$ , and (c) after heat treatment in Argon at  $1073\text{K}$  for  $10\text{ hours}$ .

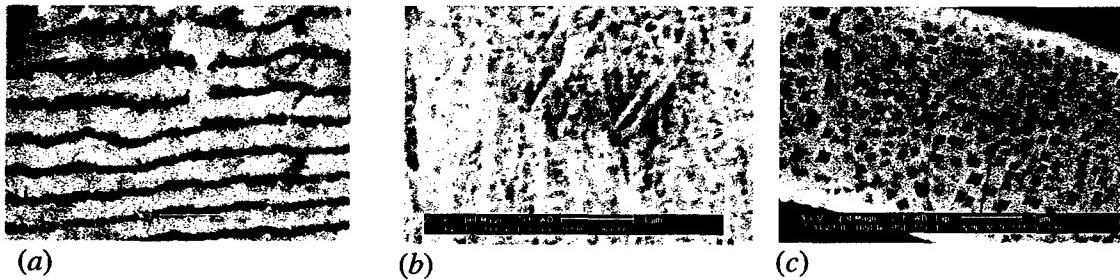


Figure 3: Cross sectional scanning electron microscope images of  $\gamma\text{-Ni(Al)}/\gamma'\text{-Ni}_3\text{Al}$  multilayers for (a)  $\Lambda = 300\text{nm}, f_{\gamma\text{-Ni(Al)}} = 0.6$  after  $1073\text{K}/10\text{ hr}$ , (b)  $\Lambda = 50\text{nm}, f_{\gamma\text{-Ni(Al)}} = 0.5$  after  $1273\text{K}/0.5\text{ hr}$ , and (c)  $\Lambda = 240\text{nm}, f_{\gamma\text{-Ni(Al)}} = 0.5$  after  $1373\text{K}/20\text{ hr}$ .

### 3. Modeling Macroscopic Room T Yield Strength of Nanoscale Laminates

Figure 4 shows design maps of the macroscopic biaxial tensile stress to yield both phases of a  $\gamma$ -Ni(Al)/ $\gamma'$ -Ni<sub>3</sub>Al nanoscale laminate, as a function of the bilayer thickness  $\Lambda$  and volume fraction  $f_{\gamma\text{-Ni(Al)}}$ . The results are based on a continuum mechanics formulation of a composite laminate with the assumptions that (1) local yield of individual layers is controlled by confined layer slip of dislocations rather than source availability and (2) macroscopic yield occurs when the applied, in-plane, biaxial stress reduced the compressive stress state in alternating layers to zero.

*Principal Result 4: Continuum modeling suggests that decreasing bi-layer thickness is a limited approach to increasing the tensile yield strength of nanoscale laminates, valid only down to a critical  $\Lambda$ . Below that, decreasing the volume fraction of the compressively stressed phase ( $\gamma'$ ) is predicted to be most effective [L3]. This result suggests a new strategy by which the plastic strength of multilayer thin films can be optimized.*

References [G6, G9] provide additional information related to Principal Result 4.

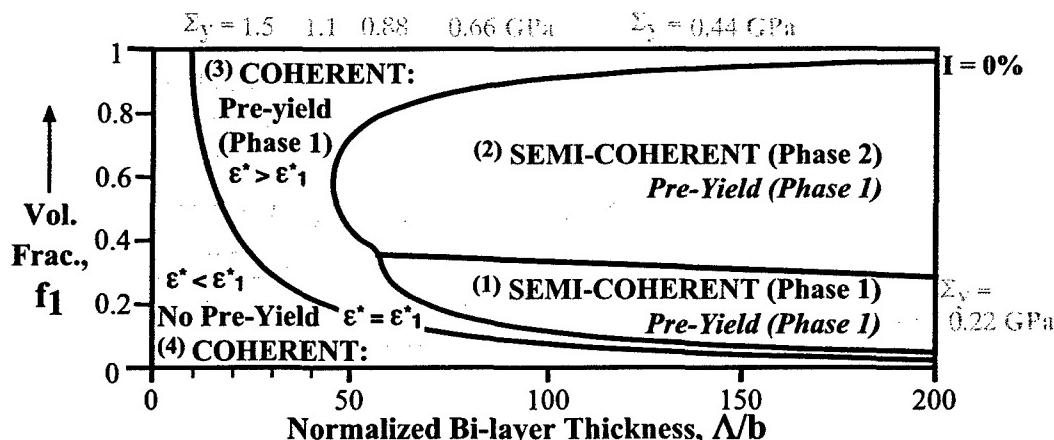


Figure 4: Predictions of the macroscopic biaxial yield strength  $\Sigma_y$  of  $\gamma$ -Ni(Al)/ $\gamma'$ -Ni<sub>3</sub>Al nanoscale laminates as a function of bilayer thickness  $\Lambda$  and volume fraction  $f_{\gamma\text{-Ni(Al)}}$ .

### 4. Discrete Dislocation Modeling of Room T Yield Strength of Nanoscale Laminates

Discrete dislocation modeling described in previous progress reports has been continued to model the biaxial yield strength of nanoscale laminates as a function of lattice parameter mismatch and bilayer thickness [L4]. As an example, Figure 5 shows the predicted critical resolved shear stress as a function of bilayer thickness for the Ag/Al system.

*Principal Result 5: Discrete dislocation modeling supports the continuum modeling observation that decreasing bi-layer thickness is a limited approach to increasing the tensile yield strength of nanoscale laminates, valid only down to a critical  $\Lambda$ . The discrete modeling predicts that a plateau in yield strength is reached with decreasing  $\Lambda$  simply because at sufficiently small  $\Lambda$ , nanoscale laminates are unable to confine dislocations to individual layers during straining [L4].*

References [G5, G7, G14, G15, G4, G19, and G20] provide additional information related to Principal Result 5.

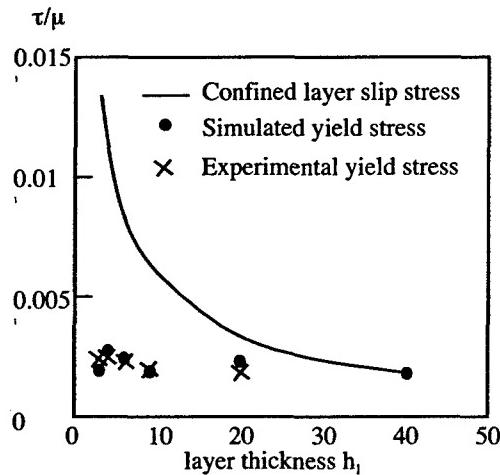


Figure 5: Critical resolved shear stress on a  $\{111\}$  slip plane in the Ag/Al nanoscale laminate system as a function of individual layer thickness,  $h = h_{\text{Ag}} = h_{\text{Al}}$ , normalized by Burgers vector magnitude  $b$ . Filled circles show the predicted value from the discrete dislocation code with a core cutoff parameter  $\rho = 0.05b$ , zero elastic modulus mismatch, and stress-free lattice parameter ratio  $a^0_{\text{Ag}}/a^0_{\text{Al}} = 1.009$ . Symbols 'x' indicate experimental values.

## 5. Continuum Modeling of Thermal Grooving in Nanoscale Multilayers

During the past year, we developed an extension to the Thouless treatment of thermal grooving of single films on substrates [L5], to treat thermal grooving in nanoscale laminates at elevated temperature under a constant in-plane strain rate. Figure 6a shows the resulting predictions for the evolution of a thermal groove in an aligned geometry and Figure 6b shows the corresponding evolution in a staggered grain boundary geometry. Figure 7 shows a master plot of the time to pinch off as a function of grain aspect ratio  $h_0/L_0$  and equilibrium grooving slope  $m$ .

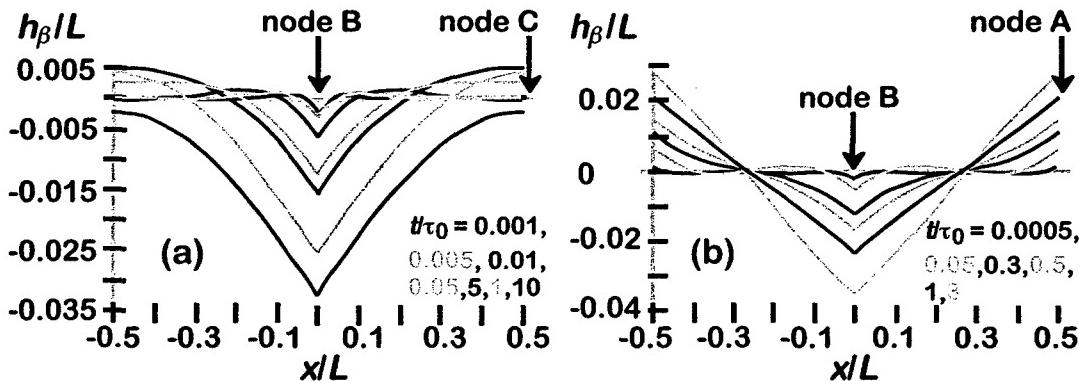


Figure 6: Evolution of the interface profile with position and time for the (a) *aligned* and (b) *staggered* configurations. The vertical position is measured relative to the initial (flat) interface. Material and geometric parameters are provided in Table 1.

**Table 1: Parameters used for simulations unless noted otherwise**

$L_0$ :	$10^{-6}$ m	$h_{\alpha(0)} = h_{\beta(0)}$ :	$10^{-6}$ m
$\gamma_{\text{int}}$ :	$1 \text{ J/m}^2$	$(D\delta)_{\text{int}}^a = 2(D\delta)_{\text{int}}^b$ :	$2 \cdot 10^{-22} \text{ m}^3/\text{s}$
$m_A = m_B$ :	0.1	$\Omega^a = \Omega^b$ :	$1 \cdot 10^{-29} \text{ m}^3/\text{atom}$
$T$ :	600 K	$\dot{\varepsilon}_{\infty}$ :	$10^{-6}/\text{s}$

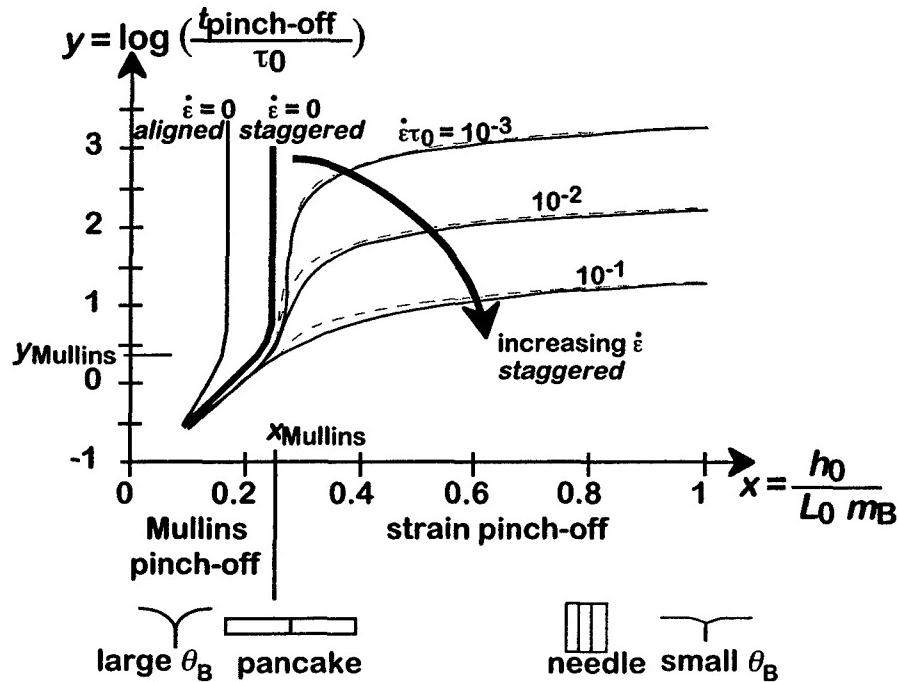


Figure 7: Time to pinch off  $\beta$  phase at node B, as a function of initial grain aspect ratio  $h_0/L_0$  and grooving slope  $m_B$ , for the aligned geometry with  $\dot{\varepsilon}_{\infty} = 0$ , and for the staggered geometry with  $m_A = m_B$  and  $\dot{\varepsilon}_{\infty} \geq 0$ . Thinner black lines for  $\dot{\varepsilon}_{\infty} > 0$  show numerical results based on Eq. 19 and dashed curves show approximate results using Eq. 36.

*Principal Result 6: Thermal grooves for nanoscale laminates should exhibit the same stability as for micron-scale laminates, provided a microstructural parameter  $x$  representing the aspect ratio of columnar grains and equilibrium grooving angle remains greater than a critical value indicated in Figure 7. If the microstructural parameter  $x$  is less than the critical value, nanoscale laminates will pinch off at  $10^{12}$  times that for micron scale laminates, since the kinetic time scale for pinch-off scales as (in-plane grain size)<sup>4</sup>. Columnar grains with a needle-like aspect ratio or shallow grooving angle are predicted to be more stable to pinch-off than grains with a pancake-like aspect ratio or large grooving angle.*

References [G1, G21] provide additional information related to Principal Result 6.

## E. ACKNOWLEDGEMENT/DISCLAIMER

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endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.

#### F. PERSONNEL SUPPORTED

1. Peter M. Anderson Assoc. Prof., MSE, Ohio State University
2. Evan Sperling MS Student, MSE, Ohio State University
3. Adrienne Lamm MS Student, MSE, Ohio State University
4. Qizhen Li PhD Student, MSE, Ohio State University
5. Yao Shen PhD, MSE, Ohio State University

#### G. PUBLICATIONS (THESE WERE SUPPORTED IN WHOLE OR IN PART BY THIS PROJECT)

2004

1. Anderson PM, Wang J, Narayanaswamy S, "Thermal Grooving in Single versus Multilayer Thin Films", **MRS Symposium Proceedings 854E** (Vinci RP, Schwaiger R, Karim A, Shenoy V, eds), pp. U7.4.1-U7.4.6, Materials Research Society: Warrendale, PA (2004). Blue Ribbon Award Winner
2. Anderson PM, Foecke T, Misra A, Rudd RE (eds), "Nanoscale Materials and Modeling: Relations Among Processing, Microstructure, and Mechanical Properties", **MRS Proceedings Volume 821**, Materials Research Society (Warrendale, PA; USA) 2004.
3. Sperling EA, Anderson PM, Hay JL, "Correlation of Stress State and Nanohardness Via Heat Treatment of Nickel-Aluminide Multilayer Thin Films", **Journal of Materials Research 19** (11) 3374-3381 (2004).
4. Shen Y, Anderson PM, "A 2D Peierls Model for Screw Dislocation Transmission across a Coherent Interface", **TMS Letters 1**(1) 17-18 (2004).
5. Li Q, Anderson PM, "A 3D Cellular Automaton Model of Dislocation Motion in FCC Crystals", **Modelling and Simulation in Materials Science and Engineering 12**, 929-943 (2004).
6. Lamm AV, Anderson PM, "Yield Maps for Nanoscale Metallic Multilayers", **Scripta Materialia 50**(6) 757-761 (2004).
7. Li Q, Anderson PM, "Dislocation Confinement and Ultimate Strength in Nanoscale Metallic Multilayers", **MRS Symposium Proceedings 791** (R. Krishnamoorti, E. Lavernia, I. Ovid'ko, C.S. Pande, G. Skandan, eds), pp. Q5.19.1-Q.5.19.6, Materials Research Society: Warrendale, PA (2004).
8. Li Q, Mills MJ, Anderson PM, "Dislocation Confinement and Ultimate Strength in Nanoscale Polycrystals", **MRS Symposium Proceedings 791** (Krishnamoorti R, Lavernia E, Ovid'ko I, Pande CS, Skandan G, eds), pp. Q3.9.1-Q3.9.6, Materials Research Society: Warrendale, PA (2004).

2003

9. Lamm AV, Anderson PM, "Strength Design Maps for Nanolayered Composites", in "Processing and Properties of Structural Nanomaterials (Shaw LL, Suryanarayana C, Mishra RS, eds), pp. 27-34, TMS: Warrendale, PA (2003).
10. Anderson PM, Bingert JF, Misra A, Hirth JP, "Rolling Texture in Nanoscale Cu/Nb Multilayers", **Acta Materialia 51**, 6059-6075 (2003).

11. Sperling EA, Banerjee R, Thompson GB, Fain JP, Anderson PM, Fraser HL, "Processing and Microstructural Characterization of Sputter Deposited Ni/Ni<sub>3</sub>Al Multilayer Thin Films", **Journal of Materials Research** **18** (4), 797-987 (2003).
  12. Banerjee R, Thompson GB, Anderson PM, Fraser HL, "Sputter-Deposited Nanocrystalline Ni-25Al Alloy Thin Films and Ni/Ni<sub>3</sub>Al Multilayers", **Thin Solid Films** **424** (1), 93-98 (2003).
  13. Mitchell TE, Anderson PM, Baskes MI, Chen SP, Hoagland RG, Misra A, "Nucleation of Kink Pairs on Partial Dislocations: a New Model for Solution Hardening and Softening", **Philosophical Magazine** **83**(11), 1329-1346 (2003).
- 2002
14. Anderson PM, Li Q, "Computer Modeling of Dislocation Motion in Fine-Scale Multilayer Composites", in **Modeling the Performance of Engineering Structural Materials III** (Lesuer DR, Srivatsan TS, Taleff EM, eds), pp.237-251, TMS: Warrendale, PA (2002).
  15. Shen C, Kazaryan A, Anderson PM, Wang Y, "Phase Field Modeling of Dislocation-Impurity and Dislocation-Precipitate Interactions", Tech. Proc. 2002 Int. Conf. Comp. Nanoscience and Nanotech., ICCN 2002, Appl. Comp. Res. Soc., Cambridge, MA (2002), pp. 259-262.
  16. Thompson GB, Banerjee R, Zhang XD, Anderson PM, Fraser HL, "Chemical Ordering and Texture in Sputter-deposited Ni<sub>3</sub>Al Thin Films", **Acta Materialia** **50**(3), 643-651 (2002).
- 2001
17. Li Qizhen, Anderson PM, "A Compact Solution for the Stress Field of a Transforming Cuboidal Particle Based on Dislocation Theory", **Journal of Elasticity** **64**, 237-245 (2001). MathCad programs are available for download that calculate the stress field around an embedded cuboidal particle undergoing a shear or direct strain transformation.
  18. Banerjee R, Fain J, Anderson PM, Fraser HL, "Influence of Crystallographic Orientation and Layer Thickness on the Fracture Behavior of Ni/Ni<sub>3</sub>Al Thin Films", **Scripta Materialia** **44**, 2629-2633 (2001).
  19. Anderson PM, Li Z, "A Peierls Analysis of the Critical Stress for Transmission of a Screw Dislocation Across a Coherent, Sliding Interface", **Materials Science Engineering A** **319-321**, 182-187 (2001).
- 2000
20. Anderson PM, Xin X, "A Peierls Approach to the Critical Shear Stress for Dislocation Transmission Through a Bi-material Interface", **James R Rice 60th Anniversary Volume** (Chuang J, Rudnicki JW, eds), pp. 87-106, Kluwer Publishers: Dordrecht (2000).
  21. Fain JP, Banerjee R, Josell D, Anderson PM, Fraser H, Tymiak N, Gerberich WW, "Morphological Stability of Ni(Al)/Ni<sub>3</sub>Al Nanolaminate Composites", **MRS Symposium Proceedings** **581**, pp. 603-608, Materials Research Society: Warrendale, PA 2000.
  22. Banerjee R, Fain JP, Anderson PM, Fraser HL, "Processing, Microstructure, and Fracture Behavior of Nickel/Nickel Aluminide Multilayered Thin Films", **MRS Symposium Proceedings** **594**, pp. 19-24, Materials Research Society: Warrendale, PA (2000).

## H. INTERACTIONS/TRANSITIONS

### 1. Participation/presentations at meetings, conferences, seminars:

1. Anderson PM: "Dislocation Interactions with Multilayer Interfaces". **Gordon Research Conference** on "Thin Film and Small Scale Mechanical Behavior", Colby College, Waterville, ME, July 18-23, 2004.

2. **Anderson PM:** "Multilayer Thin Films: Strategies for Making Superhard Materials", Center for Materials Research, **Ohio State University**, Columbus, OH, May 20, 2004.
3. **Anderson PM:** Mills MJ, Ghosh S, "Quench Cracking in Ni-Base Superalloy Turbine Disks", **General Electric Corp**, Evendale, OH, April 28, 2004.
4. **Anderson PM:** "Plasticity and Strength in Multilayer Thin Films", Mechanical Engineering, **Yale University**, New Haven, CT, April 22, 2004.
5. **Narayanaswamy S**, Anderson PM, Misra A, Cox B: "Morphological Stability of Multilayer Systems", Symposium P "Nanoscale Materials and Modeling", **MRS Spring Meeting**, San Francisco, CA, April 12-16, 2004. (co-authors are research collaborators).
6. **Anderson PM**, Shen Y: "A Peierls Model of the Critical Stress to Transmit a Screw Dislocation from a Disordered to an Ordered Phase", Symposium on "Dislocations in Complex Materials", **TMS Annual Meeting**, Charlotte, VA, March 15-19, 2004. (Shen is a grad student of the nominee).
7. **Anderson PM**, Sandhage KS, Pirouz P, Bawazer L, Phillips D, Shastry K: "A Novel MEMS-Based, Combinatorial Chemistry Approach to Measure Interfacial Strengths in Advanced Materials", Joint **AFRL/DAGSI** Research Program Symposium, Wright State University, March 2, 2004. (Bawazer and Phillips are co-advised by the nominee and Sandhage; others are research collaborators).
8. **Phillips D**, Sandhage KH, Anderson PM: A Bicrystal Microcantilever Method for Evaluating the Effects of Segregants and Misorientation Angle on Interfacial Fracture Toughness, Symposium A, **MRS Fall Meeting**, Boston, MA, Nov. 30-Dec. 5, 2003. (Phillips is co-advised by the nominee and Sandhage).
9. **Li Q**, Hazzledine PM, Mills M, Anderson PM: Dislocation Confinement and Ultimate Strength in Nanoscale Polycrystals, Symposium Q, **MRS Fall Meeting**, Boston, MA, Nov. 30-Dec. 5, 2003. (Li is a grad student of the nominee; others are research collaborators).
10. **Li Q**, Anderson PM: Dislocation Confinement and Ultimate Strength in Nanoscale Metallic Multilayers, Symposium Q, **MRS Fall Meeting**, Boston, MA, Nov. 30-Dec. 5, 2003. (Li is a grad student of the nominee).
11. **Lamm AV**, Anderson PM: Design Maps for the Tensile Yield Strength of Nanoscale Metallic Multilayers, Symposium U, **MRS Fall Meeting**, Boston, MA, Nov. 30-Dec. 5, 2003. (Lamm is a grad student of the nominee).
12. **Sperling EA**, Anderson PM: Correlation of Stress State and Nanohardness in Heat Treatment of Nickel-Aluminide Multilayered Thin Films, Symposium U, **MRS Fall Meeting**, Boston, MA, Nov. 30-Dec. 5, 2003. (Sperling is a grad student of the nominee).
13. **Li Q**, Hazzledine PM, Mills MJ, Anderson PM: The Critical Stress for Dislocation Propagation from Grain Boundaries in Nanograined Materials, **TMS Fall Meeting**, Chicago, IL, Nov. 9-12, 2003. (Li is a grad student of the nominee; others are research collaborators).
14. **Lamm AV**, Anderson PM: Strength Design Maps for Nanolayered Composites, **TMS Fall Meeting**, Chicago, IL, Nov. 9-12, 2003. (Lamm is a grad student of the nominee).
15. **Anderson PM:** Nanoscale Engineering of Multilayer Laminates for High Temperature Application, AFOSR Metallic Materials Contractors' Meeting, Boulder, CO, Aug. 4, 2003.
16. **Anderson PM**, Mitchell TE, Baskes MI, Chen SP, Hoagland RG, Misra A: Solution Hardening and Softening: A New Model Based on Double Kink Nucleation on Partials, **TMS Annual Meeting**, San Diego, CA, March 2-7, 2003. (co-authors are research collaborators).
17. **Sperling EA**, Genc A, Banerjee R, Anderson PM, Fraser HL: Characterization and Mechanical Properties of Sputter-Deposited Ni<sub>3</sub>Al Thin Films, **TMS Annual Meeting**, San

- Diego, CA, March 2-7, 2003. (Sperling is a grad student of the nominee; others are research collaborators).
- 18. **Li Q**, Anderson PM: Computer Simulation of Dislocation Propagation and Interaction in Nanostructured Metallic Multilayers, **MRS Fall Meeting**, Boston, MA, December 1-4, 2002. (Li is a grad student of the nominee).
  - 19. **Misra A**, Bingert JF, Hammon DL, Hirth JP, Anderson PM, Hoagland RG, Embury JD, Nastasi M, Kung H: The Effect of Length Scale On the Deformation of metallic Multilayers—Part II: Modeling, **MRS Fall Meeting**, Boston, MA, December 1-4, 2002. (co-authors are research collaborators).
  - 20. **Anderson PM**: The Effect of Length Scale On the Deformation of Metallic Multilayers—Part II: Modeling, **MRS Fall Meeting**, Boston, MA, December 1-4, 2002.
  - 21. **Shen Y**, Anderson PM: A Peierls Model of the Critical Stress to Transmit a Screw Dislocation from a Disordered to an Ordered Phase, **TMS Fall Meeting**, Columbus, OH, October 6-10, 2002. (Shen is a grad student of the nominee).
  - 22. **Li Q**, Anderson PM: Computer Simulation of Dislocation Motion in Fine-Scale Multilayered Composites, **TMS Fall Meeting**, Columbus, OH, October 6-10, 2002. (Li is a grad student of the nominee).
  - 23. **Anderson PM**, Mitchell TE, Baskes MI, Chen SP, Hoagland RG, Misra A: A New Model Based on Double Kink Nucleation on Partials, **TMS Fall Meeting**, Columbus, OH, October 6-10, 2002.
  - 24. **Anderson PM**: Nanoscale Engineering of Multilayer Laminates for High T Application, **AFOSR Metallic Materials Contractor's Meeting**, Bar Harbor, ME, Aug. 12-14, 2002.
  - 25. **Anderson PM**, Hoagland RG: Strengthening Effects of Interfaces in Metallic Multilayer Composites, **Gordon Conference on Physical Metallurgy**, Plymouth, NH, July 21-26, 2002. (Hoagland is a research collaborator).
  - 26. **Anderson PM**, Li Q, Hoagland RG, Misra A, Foecke T, Kramer D: Dislocation Motion in Nanoscale Multilayer Films: Computer Simulations and Experimental Observations, **U.S. National Congress on Theoretical and Applied Mechanics**, Blacksburg, VA, June 23-27, 2002. (Li is a grad student of the nominee; others are research collaborators).
  - 27. Anderson PM, Sperling EA, Banerjee R, Thompson GB, Fraser HL: Morphological Stability of Sputter-Deposited Ni(Al)/Ni<sub>3</sub>Al Multilayered Thin Films, **Nano 2002: the Sixth International Conference on Nanostructured Materials**, Orlando, FL, June 16-21, 2002. (Sperling is a grad student of the nominee; others are research collaborators).
  - 28. **Anderson PM**: Of Multilayer Thin films, Particulate-Reinforced Composites, and Strong Interfaces, **MST-8 Seminar**, Los Alamos National Labs, Los Alamos, NM, Nov. 19, 2001.
  - 29. **Anderson PM**, Wang Y, Shen C, Li Q, Foecke T: Deformation in Multilayered Thin Films: Phase Field and Discrete Dislocation Modeling, **MRS Fall Meeting**, Boston, MA, Nov. 25-30, 2001. (Li is a grad student of the nominee; others are research collaborators).
  - 30. **Anderson PM**, Li Z: The Critical Stress to Transmit a Screw Dislocation: Effect of Interfacial Bonding, **TMS Fall Meeting**, Indianapolis, IN, Nov. 4-8, 2001. (Li is a grad student of the nominee).
  - 31. **Anderson PM**, Li Q: A Simplified Solution for the Stress Field of a Misfitting Cuboidal Particle, **TMS Fall Meeting**, Indianapolis, IN, Nov. 4-8, 2001. (Li is a grad student of the nominee).
  - 32. Anderson PM, Sperling EA, Banerjee R, Fraser HL: Thermal Processing of Sputter-Deposited Ni(Al)/Ni<sub>3</sub>Al Multilayer Films into Ni-Base Superalloys with a Gamma-prime

- Precipitate Morphology, **Third International Symposium on Structural Intermetallics**, Jackson Hole, WY, Sept. 23-27, 2001. (Sperling is a grad student of the nominee; others are research collaborators).
- 33. **Anderson PM**, Fraser HL, Li Z, Sperling EA, Hazzledine PM: Nanoscale Engineering of Multilayer Laminates for High T Application, **AFOSR Metallic Materials Contractor's Meeting**, Snowbird, UT, Aug. 20-21, 2001. (Li and Sperling are grad students of the nominee; others are research collaborators).
  - 34. **Sperling EA**: Anderson PM, Thermal Stability of Nanoscale Multilayers, **Denman Graduate Research Forum**, Ohio State University, May 21, 2001. (Sperling is a grad student of the nominee).
  - 35. **Anderson PM**: Computer Modeling of Crystal Slip and Diffusional Transport in Polycrystals, Plasticity Workshop, **UES Inc.**, Dec. 6, 2000.
  - 36. **Anderson PM**: Design of Multilayer Thin Films for Optimal Strength, **Brown University Joint Materials/Solid Mechanics Seminar**, Dec. 4, 2000. (Li is a grad student of the nominee).
  - 37. **Anderson PM**, Li Z: The Ultimate Strength in Multilayer Thin Films, **MRS Symp. on The Limits of Strength in Theory and Practice**, **MRS Fall Meeting**, November 29, 2000. (Li is a grad student of the nominee).
  - 38. **Anderson PM**, Foecke T: Deformation Mechanisms in Single Crystal Metallic Nanolaminates: Theory and Experiment, **MRS Symp on Structure and Mechanical Properties of Nanophase Materials--Theory and Computer Simulations vs Experiment**, **MRS Fall Meeting**, November 29, 2000. (Foecke is a research collaborator).
  - 39. **Anderson PM**, Glaser E, Veress A, Pharr G, Vince G, Cornhill JF, Herderick E: Using Indentation and Intra-Vascular Ultrasound to Measure Arterial Response, **MRS Symp on Cardiovascular Biomaterials**, **MRS Fall Meeting**, November 28, 2000. (Glaser and Veress are co-advised by the nominee and JF Cornhill; others are research collaborators).
  - 40. **Anderson PM**: Deformation Mechanisms in Multilayered Materials, **AFOSR Metallic Materials Meeting**, St. Louis, MO, Oct. 12, 2000.
  - 41. **Anderson PM**, Li Z: A Peierls Analysis of the Critical Stress for Transmission of a Screw Dislocation Across a Coherent, Sliding Interface, **International Conference on Strength of Materials**, Asilomar, CA, Aug. 29, 2000. (Li is a grad student of the nominee).

## **2. Consultive and Advisory Functions to Other Labs/Agencies:**

- 1. Dr. Fraser has served on the Materials and Structures Panel of the USAF Scientific Advisory Board, involving reviewing of the Materials and Structures programs of AFOSR and Materials Directorate of Wright Facility, Materials Directorate (WL/ML). He has also consulted for the Characterization Facility, Materials Directorate (WL/ML).
- 2. Dr. Anderson has continued to serve as a reviewer of proposals for DOD and NSF Agencies and has interacted on multilayered systems with Dr. P. Hazzledine at UES, Inc., Drs. Tim Foecke and Dan Josell at NIST, and Drs. Amit Misra, Richard Hoagland, and Terry Mitchell at Los Alamos National Laboratory.

## **I. AWARDS RECEIVED**

- 1. October 2001-June 2002. Bernd T. Matthias Fellow at Los Alamos National Laboratory. (Only one recipient is selected per year, based on an internal review by the Materials Science and Technology Division and approval of the Laboratory Director at Los Alamos National

- Laboratory. Past recipients include David Turnbull, Ronal Gibala, J David Embury, Rishi Raj, C Barry Carter.)
2. July 21-26, 2002. Invited Speaker, Gordon Research Conference on Physical Metallurgy, Plymouth, NH.
  3. July 18-23, 2004. Invited Speaker, Gordon Research Conference on "Thin Film and Small Scale Mechanical Behavior", Colby College, Waterville, ME.
  4. April, 2005. Recipient, Lumley Award for Excellence in Research, College of Engineering, Ohio State University. This award was made based on research from 2000 to 2005 which includes research sponsored by this AFOSR project.

#### **J. TRANSITIONS**

1. **Yield\_Map\_v1.mcd:** A downloadable version of the design software is offered at:  
[http://mse-pma1.eng.ohio-state.edu/~peterand/software/yield\\_map\\_v1.mcd](http://mse-pma1.eng.ohio-state.edu/~peterand/software/yield_map_v1.mcd)  
This software is a MathCad-based program that computes yield maps for A/B multilayer thin film systems loaded in biaxial tension and which have a cube-on-cube epitaxial orientation relation between A and B phases.
2. **Shear.mcd:** A downloadable version of software is offered at:  
<http://mse-pma1.eng.ohio-state.edu/~peterand/software/shear.mcd>  
This software is a MathCad-based program that computes the stress distribution around a cuboidal inclusion that undergoes a shear transformation in an elastically-deforming matrix.
3. **Direct.mcd:** A downloadable version of software is offered at:  
<http://mse-pma1.eng.ohio-state.edu/~peterand/software/direct.mcd>  
This software is a MathCad-based program that computes the stress distribution around a cuboidal inclusion that undergoes a direct (extensional) transformation in an elastically-deforming matrix.

#### **K. STUDENTS GRADUATED UNDER SPONSORSHIP FROM THIS PROJECT**

1. Yao Shen, Ph.D. A Peierls Model of Dislocation Transmission Through Coherent Interfaces and Embedded Layers. 2004.
2. Qizhen Li, Ph.D., Theory and Modeling of the Mechanical Behavior of Nanoscale and Fine-scale Multilayer Thin Films. 2004.
3. Ziyong Li, M.S., The Critical Shear Stress for Transmission of a Peierls Screw Dislocation Across a Sliding Interface. 2001.
4. Evan Sperling, Processing, Mechanical Properties, and Morphological Stability of Ni(Al)/Ni<sub>3</sub>Al Multilayered Thin Films. 2003.
5. Adrienne Lamm, Dislocation Modeling of Mechanical Properties of Nanolayered Composite Materials. 2004.

#### **L. REFERENCES**

1. E.A. Sperling, Processing, Mechanical Properties, and Morphological Stability of Ni(Al)/Ni<sub>3</sub>Al Multilayered Thin Films, M.S. Thesis, Ohio State University, June 2003.
2. E.A. Sperling, R. Banerjee, G.B. Thompson, J.P. Fain, P.M. Anderson, and H.L. Fraser, Processing and Microstructural Characterization of Sputter Deposited Ni/Ni<sub>3</sub>Al Multilayer Thin Films, Journal of Materials Research, 2003, 18(4): 797-987.

3. A.V. Lamm and P.M. Anderson, Yield Maps for Nanoscale Metallic Multilayers, accepted *Scripta Materialia* (June 2003).
4. P.M. Anderson and Q. Li, Computer Modeling of Dislocation Motion in Fine-Scale Multilayer Composites, in *Modeling the Performance of Engineering Structural Materials III* (D.R. Lesuer, T.S. Srivatsan, and E.M. Taleff, ed), TMS, Warrendale, PA, 2002, 237-251.
5. M.D. Thouless, Effect of Surface Diffusion on the Creep of Thin-Films and Sintered Arrays of Particles, *Acta Metallurgica et Materialia*, 1993, 41: 1057-64.

## REPORT OF INVENTIONS AND SUBCONTRACTS

*(Pursuant to "Patent Rights" Contract Clause) (See Instructions on back)*

The public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed and completing and reviewing the collection of information, including suggestions for reducing the burden. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing the burden to the Department of Defense, Executive Services and OMB control number.

**PLEASE DO NOT RETURN YOUR COMPLETED FORM TO THE ABOVE ORGANIZATION. RETURN COMPLETED FORM TO THE CONTRACTING OFFICER.**

1.a. NAME OF CONTRACTOR/SUBCONTRACTOR Anderson, Peter M.	c. CONTRACT NUMBER same as 2(c)	2.a. NAME OF GOVERNMENT PRIME CONTRACTOR AFOSR/PKC	c. CONTRACT NUMBER F49620-01-1-0092	3. TYPE OF REPORT (X one) <input checked="" type="checkbox"/> a. INTERIM <input type="checkbox"/> b. FINAL
b. ADDRESS (Include Zip Code) Dept. MSE, Ohio State University 2041 College Road, Columbus, OH 43210-1179	d. AWARD DATE (YYYY/MM/DD) 2000/07/01	b. ADDRESS (Include Zip Code) 875 North Randolph St, Suite 325, Room 3112, Arlington, VA 22203	d. AWARD DATE (YYYY/MM/DD) 2000/07/01	4. REPORTING PERIOD (YYYY/MM/DD) <input checked="" type="checkbox"/> a. FROM 2000/12/01 <input type="checkbox"/> b. TO 2004/07/31

### SECTION I - SUBJECT INVENTIONS

5. "SUBJECT INVENTIONS" REQUIRED TO BE REPORTED BY CONTRACTOR/SUBCONTRACTOR (If "None," so state)

NAME(S) OF INVENTOR(S) (Last, First, Middle Initial)	TITLE OF INVENTION(S)	DISCLOSURE NUMBER, PATENT APPLICATION SERIAL NUMBER OR PATENT NUMBER c.	ELECTION TO FILE PATENT APPLICATIONS (X)		CONFIRMATORY INSTRUMENT OR ASSIGNMENT FORWARDED TO CONTRACTING OFFICER (X)	
			(1) UNITED STATES	(2) FOREIGN	(a) YES	(b) NO
a. Anderson, Peter M.	b. NONE					

f. EMPLOYER OF INVENTOR(S) NOT EMPLOYED BY CONTRACTOR/SUBCONTRACTOR

(1) (a) NAME OF INVENTOR (Last, First, Middle Initial)	(2) (a) NAME OF INVENTOR (Last, First, Middle Initial)	g. ELECTED FOREIGN COUNTRIES IN WHICH A PATENT APPLICATION WILL BE FILED
(b) NAME OF EMPLOYER	(1) TITLE OF INVENTION	(2) FOREIGN COUNTRIES OF PATENT APPLICATION
(c) ADDRESS OF EMPLOYER (Include Zip Code)	(c) ADDRESS OF EMPLOYER (Include Zip Code)	

### SECTION II - SUBCONTRACTS (Containing a "Patent Rights" clause)

6. SUBCONTRACTS AWARDED BY CONTRACTOR/SUBCONTRACTOR (If "None," so state)	NAME OF SUBCONTRACTOR(S)	ADDRESS (Include Zip Code)	SUBCONTRACT NUMBER(S) c.	FAR "PATENT RIGHTS" d. (1) CLAUSE NUMBER	DESCRIPTION OF WORK TO BE PERFORMED UNDER SUBCONTRACT(S) e.	SUBCONTRACT DATES (YYYY/MM/DD) f.
	b. NONE					(1) AWARD
						(2) ESTIMATED COMPLETION

### SECTION III - CERTIFICATION

7. CERTIFICATION OF REPORT BY CONTRACTOR/SUBCONTRACTOR (Not required if: (X as appropriate))	SMALL BUSINESS OR NONPROFIT ORGANIZATION
I certify that the reporting party has procedures for prompt identification and timely disclosure of "Subject Inventions," that such procedures have been followed and that all "Subject Inventions" have been reported.	
a. NAME OF AUTHORIZED CONTRACTOR/SUBCONTRACTOR Peter M. Anderson	b. TITLE Associate Professor
	c. SIGNATURE Peter M. Anderson
	d. DATE SIGNED 2005/04/21

## DD FORM 882 INSTRUCTIONS

### GENERAL

This form is for use in submitting INTERIM and FINAL invention reports to the Contracting Officer and for use in reporting the award of subcontracts containing a "Patent Rights" clause. If the form does not afford sufficient space, multiple forms may be used or plain sheets of paper with proper identification of information by item number may be attached.

An INTERIM report is due at least every 12 months from the date of contract award and shall include (a) a listing of "Subject Inventions" during the reporting period, (b) a certification of compliance with required invention identification and disclosure procedures together with a certification of reporting of all "Subject Inventions," and (c) any required information not previously reported on subcontracts containing a "Patent Rights" clause.

A FINAL report is due within 6 months if contractor is a small business firm or domestic nonprofit organization and within 3 months for all others after completion of the contract work and shall include (a) a listing of all "Subject Inventions" required by the contract to be reported, and (b) any required information not previously reported on subcontracts awarded during the course of or under the contract and containing a "Patent Rights" clause.

While the form may be used for simultaneously reporting inventions and subcontracts, it may also be used for reporting, promptly after award, subcontracts containing a "Patent Rights" clause.

Dates shall be entered where indicated in certain items on this form and shall be entered in six or eight digit numbers in the order of year and month (YYYYMM) or year, month and day (YYYYMMDD). Example: April 1999 should be entered as 199904 and April 15, 1999 should be entered as 19990415.

1.a. Self-explanatory.

1.b. Self-explanatory.

1.c. If "same" as item 2.c., so state.

1.d. Self-explanatory.

2.a. If "same" as Item 1.a., so state.

2.b. Self-explanatory.

2.c. Procurement Instrument Identification (PII) number of contract (DFARS 204.7003).

2.d. through 5.e. Self-explanatory.

5.f. The name and address of the employer of each inventor not employed by the contractor or subcontractor is needed because the Government's rights in a reported invention may not be determined solely by the terms of the "Patent Rights" clause in the contract.

Example 1: If an invention is made by a Government employee assigned to work with a contractor, the Government rights in such an invention will be determined under Executive Order 10096.

Example 2: If an invention is made under a contract by joint inventors and one of the inventors is a Government employee, the Government's rights in such an inventor's interest in the invention will also be determined under Executive Order 10096, except where the contractor is a small business or nonprofit organization, in which case the provisions of 35 U.S.C. 202(e) will apply.

5.g.(1) Self-explanatory.

5.g.(2) Self-explanatory. With the exception that the contractor or subcontractor shall indicate, if known at the time of this report, whether applications will be filed under either the Patent Cooperation Treaty (PCT) or the European Patent Convention (EPC). If such is known, the letters PCT or EPC shall be entered after each listed country.

6.a. Self-explanatory.

6.b. Self-explanatory.

6.c. Self-explanatory.

6.d. Patent Rights Clauses are located in FAR 52.227.

6.e. Self-explanatory.

6.f. Self-explanatory.

7. Certification not required by small business firms and domestic nonprofit organizations.

7.a. through 7.d. Self-explanatory.

## REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-05-

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1. REPORT DATE (DD-MM-YYYY) April 21, 2005	2. REPORT TYPE Final Technical Report	3. DATES COVERED (From - To) 2000/12/01 to 2004/07/31		
4. TITLE AND SUBTITLE Nanoscale Engineering of Multilayer Laminates for High Temperature Application		5a. CONTRACT NUMBER F49620-01-1-0092		
		5b. GRANT NUMBER		
		5c. PROGRAM ELEMENT NUMBER		
		5d. PROJECT NUMBER		
		5e. TASK NUMBER		
		5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  The Ohio State University Research Foundation 1960 Kenney Road Columbus, OH 43210-1179		8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/PKC AF Office Scientific Research 875 North Randolph Street Suite 325, Room 3112 Arlington, VA 22203		10. SPONSOR/MONITOR'S ACRONYM(S)		
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)		
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.				
13. SUPPLEMENTARY NOTES				
14. ABSTRACT The aim of the proposed research as stated in the original proposal is to understand how nanoscale laminates with optimal strength, ductility, and elevated temperature stability can be engineered through the selection of component chemistry, component layer thickness, and interfacial and grain boundary structure. The first effort is to develop computational tools to model the deformation and fracture processes in nanoscale laminates based on a well-known intermetallic system. The second effort is to apply the computational tools to at least one additional laminate system.				
15. SUBJECT TERMS multilayer thin films; high temperature stability; intermetallic; computational tools				
16. SECURITY CLASSIFICATION OF:  a. REPORT 13		17. LIMITATION OF ABSTRACT c. THIS PAGE 1	18. NUMBER OF PAGES 13	19a. NAME OF RESPONSIBLE PERSON Peter M. Anderson
				19b. TELEPHONE NUMBER (include area code) (614) 292-0176